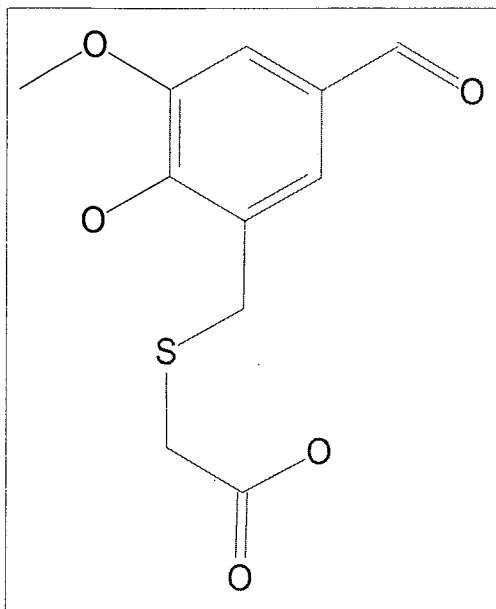


# EXHIBIT B



## Substance Identification

Beilstein Registry Number	<b>6654842</b>
Chemical Name	(5-formyl-2-hydroxy-3-methoxy-benzylsulfanyl)-acetic acid
Autoname	(5-formyl-2-hydroxy-3-methoxy-benzylsulfanyl)-acetic acid
Molecular Formula	C <sub>11</sub> H <sub>12</sub> O <sub>5</sub> S
Molecular Weight	256.27
Lawson Number	9659, 1774, 289
Type of Substance	isocyclic
Constitution ID	5733058
Tautomer ID	6297891
Beilstein Reference	6-08

## Field Availability List 1-4

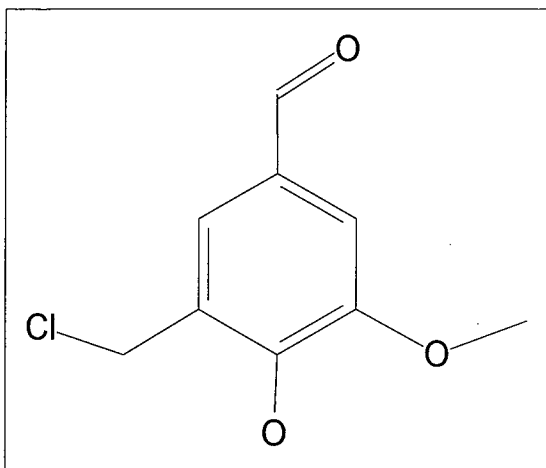
Code	Field Name	Occ.
<u><b>RX</b></u>	Reaction	2
<u><b>MP</b></u>	Melting Point	1
<u><b>NMR</b></u>	NMR Spectroscopy	2
<u><b>CNR</b></u>	Reference	1

## Reaction 1 of 2

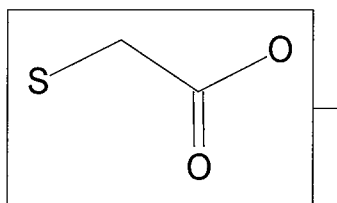
Reaction ID	<b>2901564</b>
Reactant BRN	<b>2454332</b> 3-chloromethyl-4-hydroxy-5-methoxy-benzaldehyde
	<b>506166</b> mercaptoacetic acid
Product BRN	<b>6654842</b> (5-formyl-2-hydroxy-3-methoxy-benzylsulfanyl)-acetic acid
No. of Reaction Details	1
Reaction Classification	Preparation
Yield	7 percent (BRN=6654842)
Reagent	Et <sub>3</sub> N
Solvent	CH <sub>2</sub> Cl <sub>2</sub>
Time	3 hour(s)
Other Conditions	Ambient temperature

Ref. 1

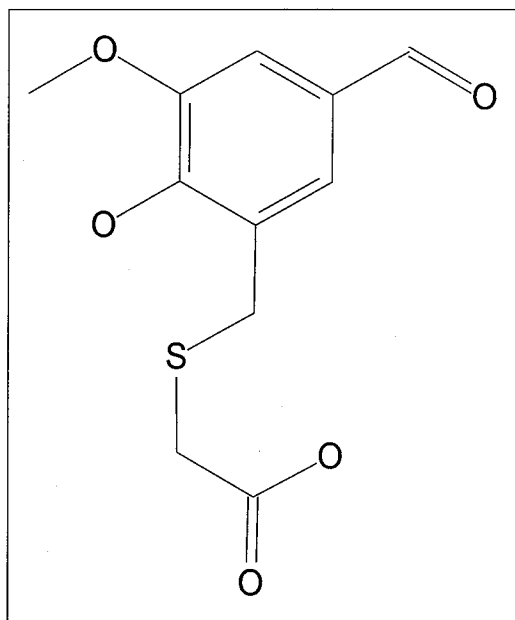
**5853919**; Journal; Gazit, Aviv; Osherov, Nir; Posner, Israel; Bar-Sinai, Allan; Gilon, Chaim; Levitzki, Alexander; JMCMAR; J. Med. Chem.; EN; 36; 23; 1993; 3556-3564.



Reactant 1



Reactant 2



Product 1

## Reaction 2 of 2

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Yield

Reagent

Solvent

Time

**3786999****6654842** (5-formyl-2-hydroxy-3-methoxy-benzylsulfanyl)-acetic acid**773697** malononitrile**6661603** [5-(2,2-dicyano-vinyl)-2-hydroxy-3-methoxy-benzylsulfanyl]-acetic acid

1.

Preparation

82 percent (BRN=6661603)

piperidine

ethanol

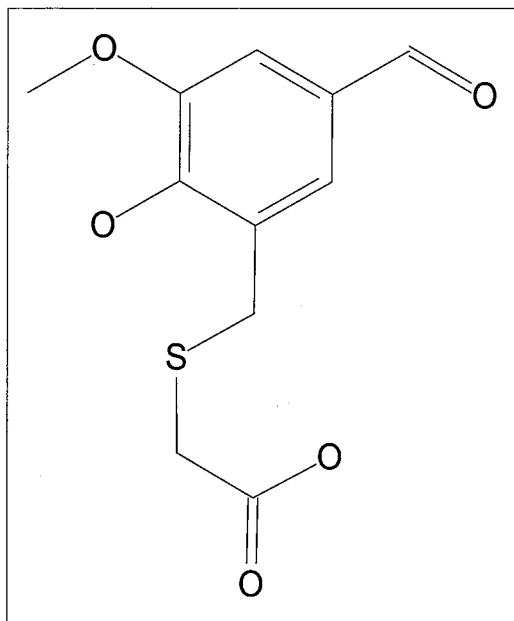
3 hour(s)

Other Conditions  
Find similar reactions

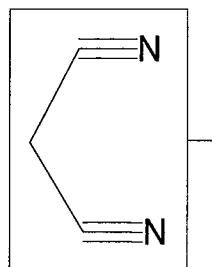
Heating  
[click here](#)

Ref. 1

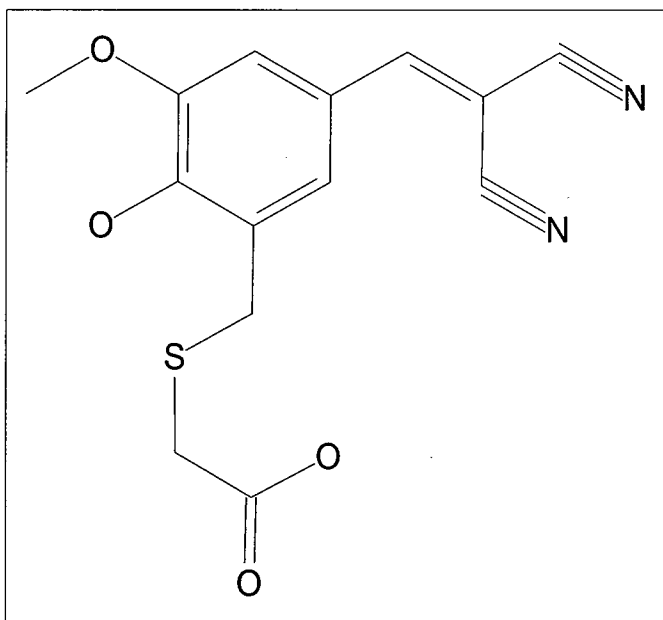
**5853919**; Journal; Gazit, Aviv; Osherov, Nir; Posner, Israel; Bar-Sinai, Allan; Gilon, Chaim; Levitzki, Alexander; JMCMAR; J. Med. Chem.; EN; 36; 23; 1993; 3556-3564.



Reactant 1



Reactant 2



Product 1

## Melting Point

VALUE (MP) C	Solvent (.SOL)	Entry Date	Note	Ref.
130				1

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Ref. 1                      **5853919**; Journal; Gazit, Aviv; Osherov, Nir; Posner, Israel; Bar-Sinai, Allan; Gilon, Chaim; Levitzki, Alexander; JMCMAR; J. Med. Chem.; EN; 36; 23; 1993; 3556-3564.

### **NMR Spectroscopy 1 of 2**

Description	Chemical shifts
Nucleus	<sup>1</sup> H
Solvents	acetone-d6

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Ref. 1                      **5853919**; Journal; Gazit, Aviv; Osherov, Nir; Posner, Israel; Bar-Sinai, Allan; Gilon, Chaim; Levitzki, Alexander; JMCMAR; J. Med. Chem.; EN; 36; 23; 1993; 3556-3564.

### **NMR Spectroscopy 2 of 2**

Description	Spin-spin coupling constants
Solvents	acetone-d6

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Note 1                      1H-1H

Ref. 1                      **5853919**; Journal; Gazit, Aviv; Osherov, Nir; Posner, Israel; Bar-Sinai, Allan; Gilon, Chaim; Levitzki, Alexander; JMCMAR; J. Med. Chem.; EN; 36; 23; 1993; 3556-3564.

### **Reference**

**5853919**; Journal; Gazit, Aviv; Osherov, Nir; Posner, Israel; Bar-Sinai, Allan; Gilon, Chaim; Levitzki, Alexander; JMCMAR; J. Med. Chem.; EN; 36; 23; 1993; 3556-3564.